Nonylphenyl diphenyl phosphate, mixed isomers
64532-97-4 | DTXSID4025797

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 54.3 °C

Global applicability domain: Inside

Local applicability domain index: 7.15e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

Image not found
Tris(3,4-dimethylphenyl) phosphate
Measured: 72.0
Predicted: 60.5

Image not found
Tris(4-methylphenyl) phosphate
Measured: 77.5
Predicted: 52.2

Image not found
Tri-m-tolyl phosphate
Measured: 25.5
Predicted: 52.1

Image not found
Triphenyl phosphate
Measured: 50.5
Predicted: 50.5

Image not found
Triphenyl phosphite
Measured: 25.0
Predicted: 36.4